

chain nodes :

11 12 13 21 22 23 24

ring nodes :

1 2 3 4 5 6 7 8 9 10 14 15 16 17 18 19

chain bonds :

2-12 3-19 4-11 12-13 13-21 21-22 21-23

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 14-15 14-19 15-16 16-17 17-18
18-19

exact/norm bonds :

1-2 1-6 2-3 3-4 3-19 4-5 4-11 12-13 13-21 21-22 21-23

exact bonds :

2-12

normalized bonds :

5-6 5-7 6-10 7-8 8-9 9-10 14-15 14-19 15-16 16-17 17-18 18-19

isolated ring systems :

containing 1 : 14 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS

=>

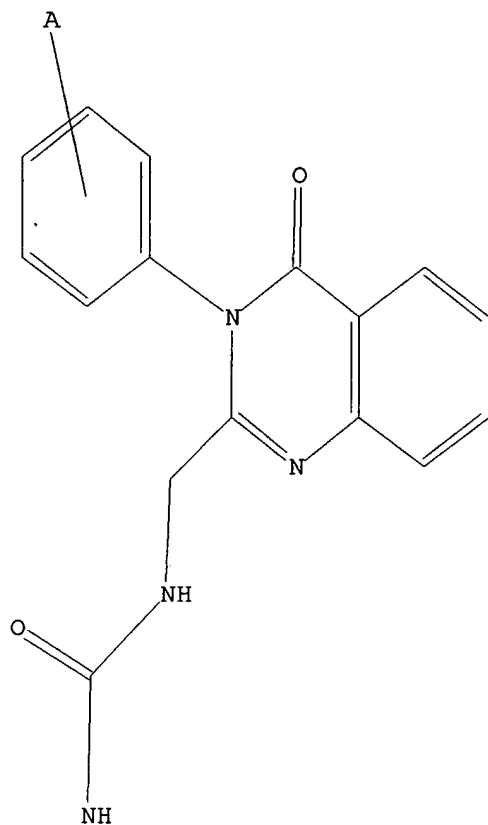
Uploading 09687800 (amended).str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 12:56:47 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 541 TO ITERATE

100.0% PROCESSED 541 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 9425 TO 12215

PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=>

Uploading 09687800 (amended).str

L3 STRUCTURE UPLOADED

=> d l3

L3 HAS NO ANSWERS

L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l3 sss sam

SAMPLE SEARCH INITIATED 12:58:06 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 540 TO ITERATE

100.0% PROCESSED 540 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 9406 TO 12194

PROJECTED ANSWERS: 1 TO 80

L4 1 SEA SSS SAM L3

=> s l3 sss ful

FULL SEARCH INITIATED 12:58:14 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 10835 TO ITERATE

100.0% PROCESSED 10835 ITERATIONS

12 ANSWERS

SEARCH TIME: 00.00.04

L5 12 SEA SSS FUL L3

=> s l5

L6 4 L5

=> d l6 1-4 bib,ab,hitstr

L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2002 ACS

AN 2001:208250 CAPLUS

DN 134:252352

TI Preparation of 3-aryl-2-aryluroidoalkylquinazolin-4-ones and related compounds as mediators of hedgehog signaling pathways.

IN Baxter, Anthony David; Boyd, Edward Andrew; Guichert, Oivin M.; Price, Stephen; Rubin, Lee D.

PA Curis, Inc., USA

SO PCT Int. Appl., 177 pp.

CODEN: PIXXD2

DT Patent

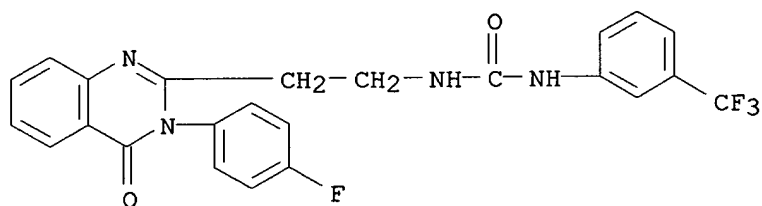
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001019800	A2	20010322	WO 2000-US25461	20000915
	WO 2001019800	A3	20011206		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
EP	1216234	A2	20020626	EP 2000-963551	20000915
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL			
PRAI	US 1999-154526P	P	19990916		
	US 1999-159412P	P	19991014		
	US 1999-162899P	P	19991101		
	WO 2000-US25461	W	20000915		
OS	MARPAT 134:252352				
AB	R1LX1Y1Z1LX2Y2Z2LR2 [R1, R2 = H, alkyl, (substituted) aryl, aralkyl, heteroaryl, heteroarylalkyl; L = null, alkyl, alkenyl, alkynyl, (CH2)nO(CH2)p, etc.; n, p = 0-10; X1, X2 = NR8, O, S, Se, N:N, ON:CH, heterocyclyl, bond, etc.; Y1, Y2 = CO, CS, SO2, SO, C(:NCN), heteroaryl, bond, etc.; Z1, Z2 = NR8, O, S, Se, N:N, ON:CH, heterocyclyl, bond, etc.; R8 = H, alkyl, (substituted) aryl, aralkyl, heteroaryl, heteroaralkyl, etc.], were prep'd. Thus, triphosgene in EtOAc was added to 4-nitro-3-trifluoromethylaniline in EtOAc followed by stirring and reflux. The mixt. was concd., dissolved in CHCl3, and treated with 3-(4-fluorophenyl)-2-(1-methylaminoethyl)-4-oxo-3,4-dihydroquinazoline in CHCl3 to give 97% 1-[1-[3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl]ethyl]-3-(3-trifluoromethyl-4-nitrophenyl)-1-methylurea. The latter inhibited sonic hedgehog-induced Gli transcription activity with IC50 <5 .mu.M.				
IT	330796-20-8P 330796-21-9P 330796-24-2P 330796-25-3P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of 3-aryl-2-aryluroidoalkylquinazolin-4-ones and related compds. as mediators of hedgehog signaling pathways)				
RN	330796-20-8 CAPLUS				
CN	Urea, N-[2-[3-(4-fluorophenyl)-3,4-dihydro-4-oxo-2-quinazolinyl]ethyl]-N'-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)				

Applicant's

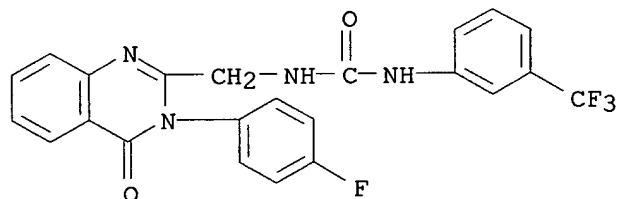
Provisional Priority Applies



*Elected
species.*

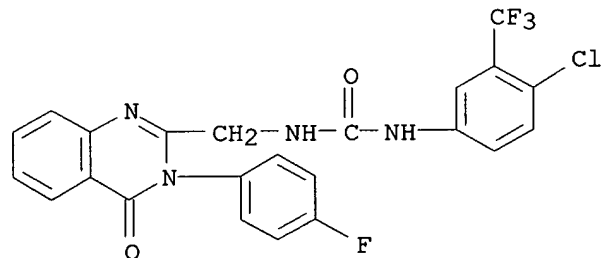
RN 330796-21-9 CAPLUS

CN Urea, N-[[3-(4-fluorophenyl)-3,4-dihydro-4-oxo-2-quinazolinyl]methyl]-N'-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



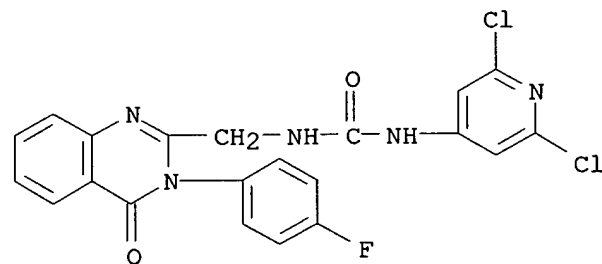
RN 330796-24-2 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[[3-(4-fluorophenyl)-3,4-dihydro-4-oxo-2-quinazolinyl]methyl]- (9CI) (CA INDEX NAME)



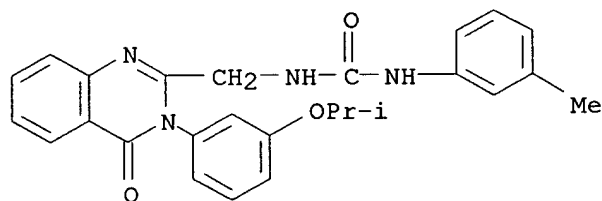
RN 330796-25-3 CAPLUS

CN Urea, N-(2,6-dichloro-4-pyridinyl)-N'-[[3-(4-fluorophenyl)-3,4-dihydro-4-oxo-2-quinazolinyl]methyl]- (9CI) (CA INDEX NAME)

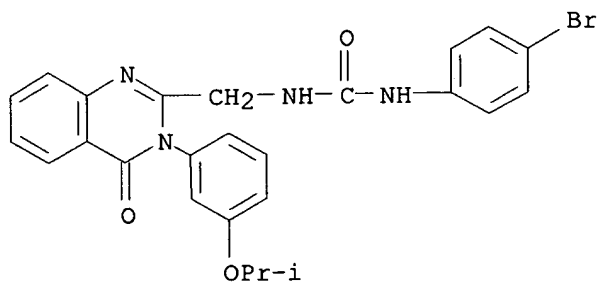


L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2002 ACS
 AN 1998:352629 CAPLUS
 DN 129:27954
 TI Quinazolinone derivatives as cholecystokinin (CCK) ligands
 IN Padia, Janak Khimchand
 PA Warner-Lambert Co., USA
 SO U.S., 23 pp., Cont.-in-part of U.S. Ser. No. 287,454.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5756502	A	19980526	US 1995-500436	19950710
	US 5869665	A	19990209	US 1997-826843	19970408
PRAI	US 1994-287454		19940808		
	US 1995-500436		19950710		
OS	CASREACT 129:27954; MARPAT 129:27954				
AB	The title compds. [I; W, X, Y, Z = CR ₃ , CR ₄ , CR ₅ , CR ₆ , N, etc.; M = O, S; B = bond or (un)substituted alkylene; A = R ₁ NCO(CH ₂) _n , CONR ₁ (CH ₂) _n , etc.; n = 0, 1; R ₁ , R ₂ = C ₁ -6 alkyl, (un)substituted aryl, etc.; R ₃ -R ₆ = H, OH, alkoxy, etc.; R ₁₁ = H, lower alkyl] are prepd. I with good binding affinity for the CCK-A and CCK-B receptors are useful agents to suppress appetite, reduce gastric acid secretion, and the like. Thus, 2-(aminomethyl)-3-[3-(methylethoxy)phenyl]-4(3H)-quinazoline (prepn. given) was reacted with 3-methylphenyl isocyanate to give 50% the title compd. (II), which showed CCK-A and CCK-B receptor binding affinities (K _i) of 1637 and 879 nm resp.				
IT	189937-54-0P 189937-57-3P 189937-58-4P 189937-60-8P 189937-63-1P 189937-64-2P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (quinazolinone derivs. as cholecystokinin (CCK) ligands)				
RN	189937-54-0 CAPLUS				
CN	Urea, N-[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2- quinazolinyl]methyl]-N'-(3-methylphenyl)- (9CI) (CA INDEX NAME)				

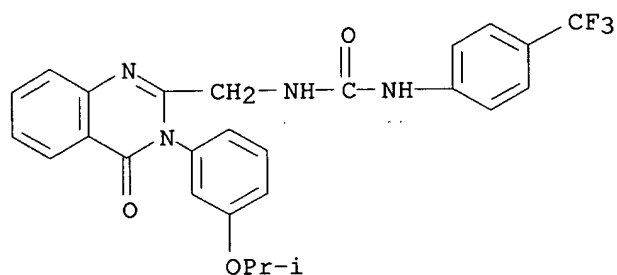


RN 189937-57-3 CAPLUS
 CN Urea, N-(4-bromophenyl)-N'-[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-
 oxo-2-quinazolinyl]methyl]- (9CI) (CA INDEX NAME)



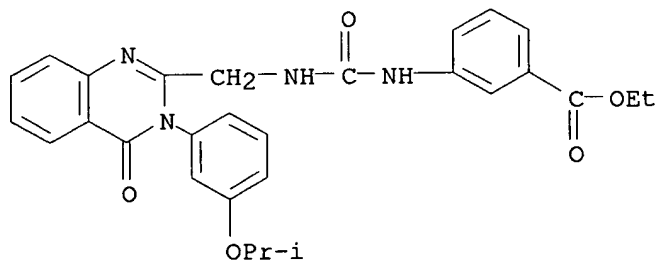
RN 189937-58-4 CAPLUS

CN Urea, N-[[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2-quinazolinyl]methyl]-N'-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 189937-60-8 CAPLUS

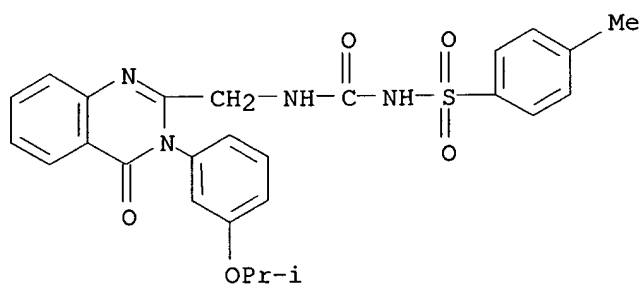
CN Benzoic acid, 3-[[[[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2-quinazolinyl]methyl]amino]carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 189937-63-1 CAPLUS

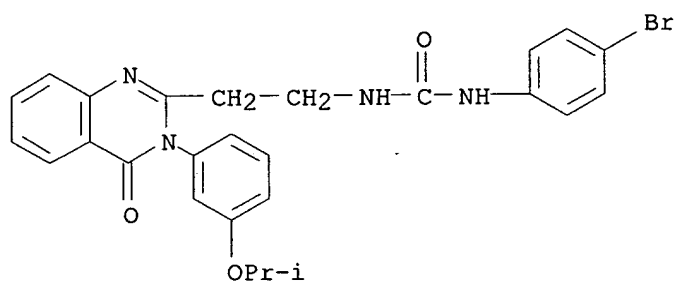
CN Benzenesulfonamide, N-[[[[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2-quinazolinyl]methyl]amino]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

09/724,277 (09/687,800)



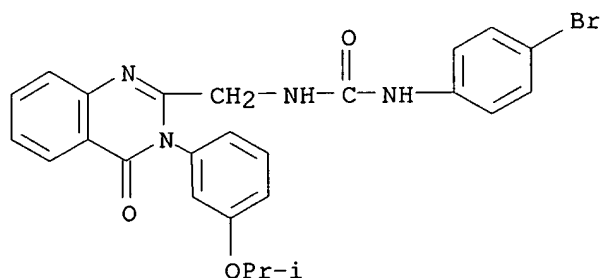
RN 189937-64-2 CAPLUS

CN Urea, N-(4-bromophenyl)-N'-[2-[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2-quinazolinyl]ethyl]- (9CI) (CA INDEX NAME)

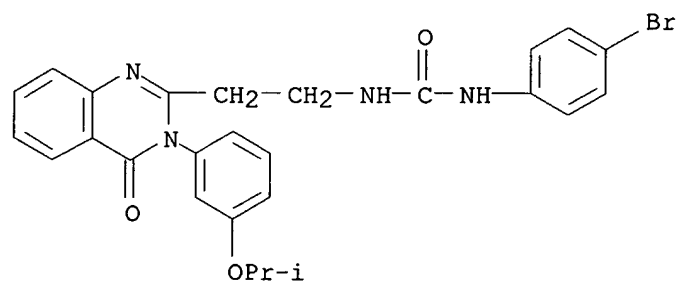


RE.CNT 83 THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

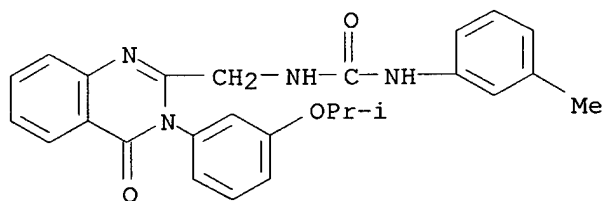
L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS
 AN 1998:169718 CAPLUS
 DN 128:238969
 TI Novel Nonpeptide CCK-B Antagonists: Design and Development of
 Quinazolinone Derivatives as Potent, Selective, and Orally Active CCK-B
 Antagonists
 AU Padia, Janak K.; Field, Mark; Hinton, Joanna; Meecham, Ken; Pablo, Julius;
 Pinnock, Rob; Roth, Bruce D.; Singh, Lakhbir; Suman-Chauhan, Nirmala;
 Trivedi, Bharat K.; Webdale, Louise
 CS Departments of Chemistry and of Pharmacokinetics and Drug Metabolism,
 Parke-Davis Pharmaceutical Research Division of Warner-Lambert Company,
 Ann Arbor, MI, 48105, USA
 SO Journal of Medicinal Chemistry (1998), 41(7), 1042-1049
 CODEN: JMCMAR; ISSN: 0022-2623
 PB American Chemical Society
 DT Journal
 LA English
 AB Urea-linked quinazolines [I; R = (un)substituted Ph, cyclohexyl; R1 =
 (un)substituted Ph, 3-pyridyl, 1-naphthyl] were prepd. as selective
 orally active CCK-B antagonists. Thus, thioxoquinazolinones II (prepd.
 from anthranilic acid and the requisite isothiocyanate) were treated with
 hydrazine gave the 2-hydrazino compds. which were then treated with an
 isocyanate to give I. Representative compds. of this series were tested
 in the functional assay, i.e., guinea pig stomach strip assay, and showed
 pure antagonist profiles. I [R = 3-(tert-butoxycarbonyl)phenyl, R1 =
 3-isopropoxyphenyl] and I [R = 3-cyanophenyl, R1 = 3-
 (dimethylamino)phenyl] (III) were orally active in the elevated rat X-maze
 test and showed dose-dependent anxiolytic-like action. These compds. were
 also evaluated for their pharmacokinetic profile. The abs. oral
 bioavailability of III was 22% in rats.
 IT **189937-57-3P 189937-64-2P**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological
 study); PREP (Preparation)
 (prepn. of urea-linked quinazolinones as selective CCK-B receptor
 antagonists)
 RN 189937-57-3 CAPLUS
 CN Urea, N-(4-bromophenyl)-N'-[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-
 oxo-2-quinazolinyl]methyl]- (9CI) (CA INDEX NAME)



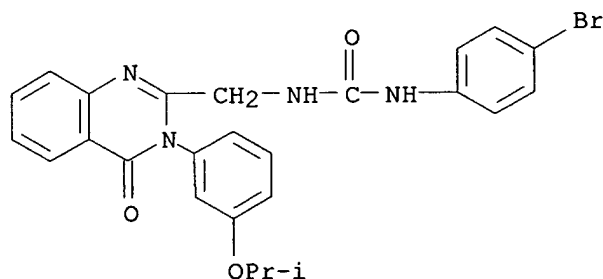
RN 189937-64-2 CAPLUS
 CN Urea, N-(4-bromophenyl)-N'-[2-[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-
 oxo-2-quinazolinyl]ethyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2002 ACS
 AN 1997:285638 CAPLUS
 DN 126:343533
 TI Design and synthesis of novel nonpeptide CCK-B receptor antagonists
 AU Padia, J. K.; Chilvers, H.; Daum, P.; Pinnock, R.; Suman-Chauhan, N.;
 Webdale, L.; Trivedi, B. K.
 CS Division of Warner-Lambert Company, Department of Chemistry, Parke-Davis
 Pharmaceutical Research, Ann Arbor, MI, 48105, USA
 SO Bioorganic & Medicinal Chemistry Letters (1997), 7(7), 805-810
 CODEN: BMCLE8; ISSN: 0960-894X
 PB Elsevier
 DT Journal
 LA English
 AB A novel hybrid series of nonpeptide CCK-B receptor antagonists,
 quinazolinones I (R = 3-Me, 4-Br, 3-CO₂Et, etc., L = CH₂, CH₂CH₂, X = O,
 S, Y = NH, NHCH₂, NHSO₂), has been designed from two known series derived
 from asperlicin. An efficient synthesis of 2-aminoquinazolinone, an
 intermediate for the synthesis of a targeted analog, has been developed.
 IT 189937-54-0P 189937-57-3P 189937-58-4P
 189937-59-5P 189937-60-8P 189937-62-0P
 189937-63-1P 189937-64-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological
 study); PREP (Preparation)
 (prepn. and CCK-B receptor antagonist activity of quinazolinones)
 RN 189937-54-0 CAPLUS
 CN Urea, N-[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2-
 quinazolinyl]methyl]-N'-(3-methylphenyl)- (9CI) (CA INDEX NAME)

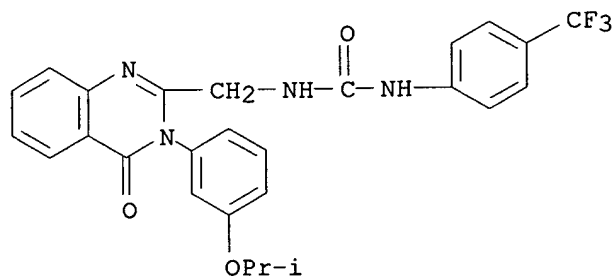


RN 189937-57-3 CAPLUS
 CN Urea, N-(4-bromophenyl)-N'-[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-
 oxo-2-quinazolinyl]methyl]- (9CI) (CA INDEX NAME)



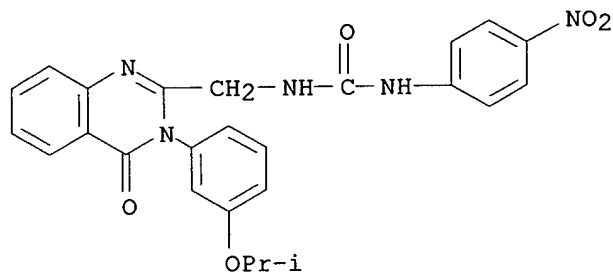
RN 189937-58-4 CAPLUS
 CN Urea, N-[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2-

quinazolinyl)methyl]-N'-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



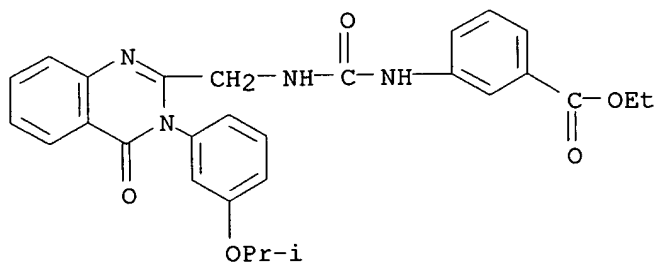
RN 189937-59-5 CAPLUS

CN Urea, N-[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2-quinazolinyl)methyl]-N'-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



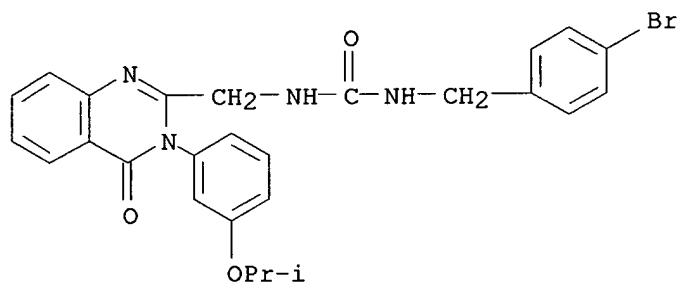
RN 189937-60-8 CAPLUS

CN Benzoic acid, 3-[[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2-quinazolinyl)methyl]amino]carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



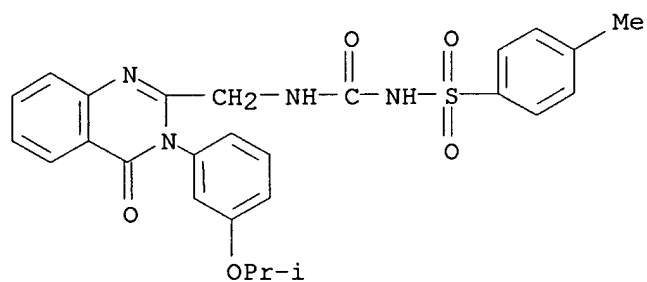
RN 189937-62-0 CAPLUS

CN Urea, N-[(4-bromophenyl)methyl]-N'-[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2-quinazolinyl)methyl]- (9CI) (CA INDEX NAME)



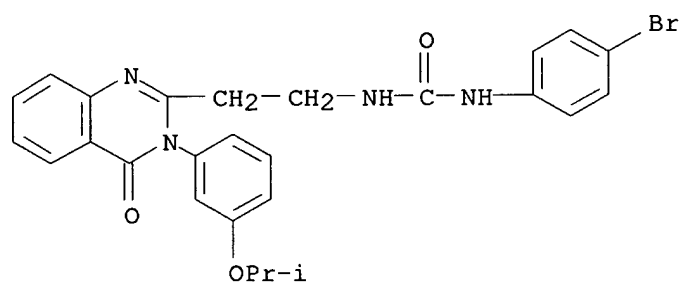
RN 189937-63-1 CAPLUS

CN Benzenesulfonamide, N-[[[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2-quinazolinyl]methyl]amino]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)



RN 189937-64-2 CAPLUS

CN Urea, N-(4-bromophenyl)-N'-[2-[3,4-dihydro-3-[3-(1-methylethoxy)phenyl]-4-oxo-2-quinazolinyl]ethyl]- (9CI) (CA INDEX NAME)



09/724,277 (09/687,800)

=> d his

(FILE 'HOME' ENTERED AT 12:56:13 ON 20 OCT 2002)

FILE 'REGISTRY' ENTERED AT 12:56:19 ON 20 OCT 2002

L1 STRUCTURE UPLOADED
L2 1 S L1 SSS SAM
L3 STRUCTURE UPLOADED
L4 1 S L3 SSS SAM
L5 12 S L3 SSS FUL

FILE 'CAPLUS' ENTERED AT 12:58:34 ON 20 OCT 2002

L6 4 S L5

FILE 'CAOLD' ENTERED AT 12:59:09 ON 20 OCT 2002

=> s l5

L7 0 L5

=> log y

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

0.38

159.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY

TOTAL
SESSION

CA SUBSCRIBER PRICE

0.00

-2.48

STN INTERNATIONAL LOGOFF AT 12:59:20 ON 20 OCT 2002